

Density Wave and Supersolid Phases of Correlated Bosons in an optical lattice

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Abstract. – Motivated by the recent experiment on the Bose-Einstein condensation of ^{52}Cr atoms with long-range dipolar interactions (Werner J. et al., Phys. Rev. Lett., 94 (2005) 183201), we consider a system of bosons with repulsive nearest and next-nearest neighbor interactions in an optical lattice. The ground state phase diagram, calculated using the Gutzwiller ansatz, shows, apart from the superfluid (SF) and the Mott insulator (MI), two modulated phases, *i.e.*, the charge density wave (CDW) and the supersolid (SS). Excitation spectra are also calculated which show a gap in the insulators, gapless, phonon mode in the superfluid and the supersolid, and a mode softening of superfluid excitations in the vicinity of the modulated phases. We discuss the possibility of observing these phases in cold dipolar atoms and propose experiments to detect them.

The recent observation [2] of quantum phase transition of interacting bosons in an optical lattice has given a new impetus to the study of correlated bosons. The possibility of manipulating both the interactions among the constituents as well as disorder in the system with extreme control, make them an ideal object over conventional solid state systems to study many-body effects. Recent experimental success in obtaining a dipolar condensate of ^{52}Cr atoms [1] opens up new directions in the study of lattice bosons with long-range interactions [3]. This also leads to the possibility of achieving new phases such as insulating charge density wave and the supersolid that has both superfluid and crystalline properties [4]. The recent experimental observation of nonclassical moment of inertia of solid ^4He indicates a possible signature of SS [5], although the existence of the SS is still a controversial issue, and we believe, the dipolar condensate in optical lattice can provide a testing ground for it.

A collection of interacting bosons on a lattice is described by the Bose-Hubbard model [6] which captures the physics arising from the competition between kinetic energy of bosons and their on-site interaction. However, long-range interactions among the dipolar bosons at different lattice sites make it necessary to include nearest-neighbor interaction in the Hamiltonian.

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The resulting extended Bose-Hubbard model (eBHM) Hamiltonian reads:

$$\hat{H} = -t \sum_{i,\delta} \hat{a}_i^\dagger \hat{a}_{i+\delta} + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + V \sum_{i,\delta} \hat{n}_i \hat{n}_{i+\delta}. \quad (1)$$

Here \hat{a}_i^\dagger creates a boson at site i , $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the boson number operator, t , U , V , are the nearest-neighbor hopping, the on-site interaction and the nearest-neighbor interaction (NNI) respectively, and δ represents the nearest neighbors of site i . This model in a high density limit, where it corresponds to a quantum phase model (QPM), has also been studied in the context of a wide variety of other problems such as Josephson junction arrays, granular superconductors, liquid ^4He in Vycor *etc.* [7, 8]. For small t , the role of NNI is to stabilize an insulating state, similar to the CDW phase in solids, where the number density alternates at every lattice site between two successive integers. In the case of soft-core bosons, it also brings in a new phase where both diagonal crystalline order and off-diagonal superfluid long-range order coexist and hence called the supersolid [4]; in this phase the number density shows a modulation, while still retaining a nonvanishing SF fraction. The model in Eq. (1) without the NNI has been extensively studied previously using different methods [6, 9, 10], and the mean-field results were found to be in good agreement with the quantum Monte-Carlo (QMC) results [9], though the critical behavior is beyond the description of the former. However, one can expect that with the increasing dimensionality d of the system, larger filling factors, and the longer range of the interactions, mean-field results will progressively become accurate. In this letter we study the eBHM using Gutzwiller mean field theory [11] to obtain the ground state phase diagram. More importantly, we extend this approach, using the time dependent variational principle, to extract the excitation spectrum of the system. This method has the added advantage of generalizing to the nonuniform systems, for example in a confining trap, which is always present in experiments. We discuss the possibility of observing these novel phases in cold atoms and propose ways to detect them.

In order to find the ground state of the Hamiltonian (1), we use the variational minimization of $\langle \Psi | \hat{H} - \mu \hat{N} | \Psi \rangle$ with a Gutzwiller wavefunction $|\Psi\rangle = \prod_i \sum_n f_n^{(i)} |n_i\rangle$ where $|n_i\rangle$ is the Fock state with n particles at site i , μ is the chemical potential, and $\hat{N} = \sum_i \hat{n}_i$ is the total particle number operator. Minimization with respect to the variational parameters $f_n^{(i)}$ gives the ground state, which could be a MI, SF, SS, or a CDW. First we consider the case when $Vd \leq U/2$. In Fig. 1, we present the phase diagram for $Vd/U = 0.4$ [12]. For small enough t , incompressible MI and CDW phases are formed. The MI phase with integer n_0 number of particles per site (denoted by $\text{MI}(n_0)$) is characterized by $f_n^{(i)} = \delta_{n,n_0}$ and a vanishing condensate order parameter $\phi_i = \sum_\delta \langle \Psi | \hat{a}_{i+\delta} | \Psi \rangle$. The CDW phase has a two sublattice periodic structure such as $n_0, n_0 - 1$ particles at the consecutive sites (denoted by $\text{CDW}(n_0/2)$) and zero ϕ_i . The SF and the SS phases have non-vanishing ϕ ; in the former it is uniform and in the latter it has a two-sublattice modulation. At small values of μ and $t = 0$, we have a $\text{CDW}(1/2)$ with $|1, 0, 1, 0\rangle$ particle density modulation. Upon further increase of μ , $\text{MI}(1)$ phase becomes energetically favourable. In general, at $t = 0$, we have transitions between $\text{CDW}(n_0/2)$ to $\text{MI}(n_0)$ at $\mu = U(n_0 - 1) + 2Vdn_0$ and then to $\text{CDW}(n_0/2 + 1)$ at $\mu = Un_0 + 2Vdn_0$. As we lower the value of V , the area of the CDW lobe reduces continuously and so is the transition point at $t = 0$ between the CDW and the MI phases; the CDW lobe vanishes completely for $V = 0$, thereby reducing to the phase diagram as in Ref. [6]. Uniform, homogeneous SF phase appears for sufficiently large values of t . In between the CDW and the SF, a supersolid (SS) phase is formed, which has a density modulation as well as nonvanishing ϕ . Here we must stress that a *finite* onsite interaction is needed, in addition to the NNI, for the existence of

checkerboard SS phase which is unstable in the hard-core limit of eBHM [13]. As t increases, the system undergoes a second-order transition from CDW(1/2) to a SS for larger values of μ (mostly for particle-doping away from half-filling) and a first order transition to SF at smaller values of μ (for hole-doping away from half-filling). A multicritical point exists at $\mu/U = 0.132$ and $td/U = 0.137$ where the two second order transition lines between SS-SF and CDW-SS meet the first order line between CDW-SF (see Fig. 1). In Fig. 2a, we plot the contours of fixed particle density as a function of μ and t for $Vd/U = 0.4$. We find the insulating lobes of fixed average commensurate densities $n_0 = 0.5$, and $n_0 = 1$ *etc.*, and SF and SS phases with incommensurate densities (in general). As shown in Fig. 2b and Fig. 2c, we observe at a given μ , the density and ϕ change continuously across CDW-SS and SS-SF transitions indicating a continuous second order transition, whereas a jump in the above quantities signals a first order transition between CDW-SF.

When $Vd > U/2$, the MI lobes vanish and the new CDW phases such as CDW(1) with a particle density modulation $|\dots, 2, 0, \dots\rangle$ appear [14]. At $t = 0$, the CDW(1/2) transforms into CDW(1) when $\mu > U$, which in turn transforms into CDW(3/2) when $\mu > 2U$. In general a $|\dots, n_0, 0, \dots\rangle$ CDW state is formed within a region $(n_0 - 1)U < \mu < n_0U$. With increasing t , the supersolid phase is formed around the CDW lobes and at still larger values of t , a homogeneous superfluid phase appears.

In 1D due to enhanced quantum fluctuations, our results differ significantly from those of the density matrix renormalization group where no SS phase was found [15]. In fact, the numerical studies of 1D BHM show that the nature of the Mott-SF phase boundary itself is quite different from that obtained from the Gutzwiller method. In 2D previous QMC studies for the hard-core ($U = \infty$) bosons found unstable checkerboard SS phase which phase separates between CDW and SF [13]. Preliminary results for the soft core bosons indicate the region of SS phase with negative compressibility [16]. However, a previous QMC study of the related quantum phase model by van Otterlo *et al.* [8] came to the conclusion that a finite U (soft core) stabilizes the checkerboard SS phase. Within the Gutzwiller approach, we find a stable SS phase over a large region of particle doping, and a relatively smaller region of SS upon hole doping the CDW, and a first order transition between the CDW and the SF below the multicritical point (region of hole doping) indicating possible phase separation. A recent QMC study *indeed* shows that a stable SS phase exists for soft-core bosons with sufficiently large values of V/U and upon particle-doping away from half-filling [17]; however, the SS obtained by hole doping turns out to be unstable with respect to phase separation. The CDW-SF transition is indeed found to be first order as expected. The region of SS phase reduces significantly with reducing V , and we expect that it will be destroyed at small enough V due to quantum fluctuations. Increasing the dimensionality to three and/or increasing the filling factor will reduce the fluctuations, thus stabilizing the SS further.

The excitation spectrum of the system can be obtained from the dynamical Gutzwiller approach with the variational parameters $f_n^{(i)}$ being time dependent. Minimization of the effective action $\langle \Psi | i \frac{\partial}{\partial t} - \hat{H} + \mu \hat{N} | \Psi \rangle$ gives the equations of motion for $f_n^{(i)}$:

$$i \frac{\partial f_n^{(i)}}{\partial \tau} = \left[\frac{U}{2} n(n-1) - \mu n + V n \rho^{(i)} \right] f_n^{(i)} - t \left(\phi_i^* \sqrt{n+1} f_{n+1}^{(i)} + \phi_i^* \sqrt{n} f_{n-1}^{(i)} \right) \quad (2)$$

where $\rho^{(i)} = \sum_{\delta, n} n |f_n^{(i+\delta)}|^2$ and τ is time. The small amplitude fluctuations $\delta f_n^{(i)}(t)$ around the ground state $\bar{f}_n^{(i)}$ give the excitation spectrum. In the MI ground state, $\delta f_n^{(i)}$ are connected only to $\delta f_{n\pm 1}^{(i)}$ in the Eq. (2). The low-lying excitations are creating particles (p) and holes (h) in the ground state with a particle density n_0 which needs a finite energy and the system is

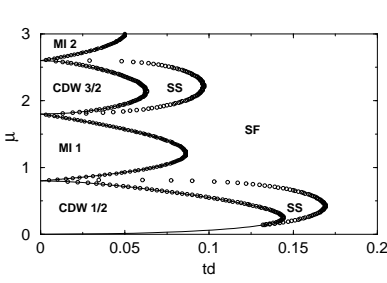


Fig. 1

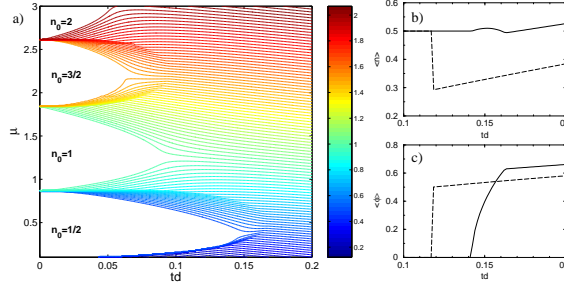


Fig. 2

Fig. 1 – Phase diagram of the eBHM for $Vd = 0.4$ (energies are in units of U). Open circles denote the numerical results and the solid lines represent the analytical results.

Fig. 2 – a) Contour plot of fixed particle density for $Vd = 0.4$ (energies are in units of U). b) Variation of the average particle density for a fixed μ and for $Vd = 0.4$. Solid line: CDW to SS to SF transition at $\mu = 0.3$. Dashed line: CDW to SF transition at $\mu = 0.1$. c) Variation of ϕ for the same parameters.

gapped. At $t = 0$, these excitations have energies $Un_0 + 2dVn_0 - \mu$ and $\mu - U(n_0 - 1) - 2dVn_0$ respectively. For nonzero t , the dispersions of these excitations are:

$$\omega_{ph} = \pm[-\epsilon/2 + U(n_0 - 1/2) + 2dVn_0 - \mu] + [(\epsilon/2)^2 - \epsilon U(n_0 + 1/2) + U^2/4]^{1/2} \quad (3)$$

where $\epsilon(\mathbf{k}) = 2t \sum_{l=1..d} \cos(k_l)$. For $V = 0$ this result agrees with the excitation spectra of the MI phase of BHM obtained within the slave boson approach [18]. In general, the CDW state has four low-lying excitations in the reduced Brillouin zone (BZ), corresponding to particle and hole excitations in each of the A (with n_1 particles per site) and B (with n_2 particles per site) sublattices. At $t = 0$, the energies of particle (hole) excitations of sublattice A are $E_A^p = Un_1 + 2dVn_2 - \mu$, $E_A^h = -U(n_1 - 1) - 2dVn_2 + \mu$, and those of sublattice B are $E_B^p = Un_2 + 2dVn_1 - \mu$, and $E_B^h = -U(n_2 - 1) - 2dVn_1 + \mu$ respectively which, as in the case of MI, pick up a dispersion at nonzero values of t . The number of particles on sublattice B is $n_2 = n_1 - 1$, for $Vd < U/2$ and $n_2 = 0$, for $Vd > U/2$. Clearly, the hole excitation in sublattice B is unphysical for $n_2 = 0$. For $Vd > U/2$, there is a qualitative change in the excitation spectrum. The excitation corresponding to a particle addition on A becomes energetically favourable compared to a particle addition on B. At finite t the excitation spectrum $\omega(\mathbf{k})$ of the insulating states can be obtained analytically by solving the algebraic equation:

$$\tilde{E}_A^p \tilde{E}_A^h \tilde{E}_B^p \tilde{E}_B^h - \epsilon^2(\mathbf{k})[(n_1 + 1)\tilde{E}_A^h + n_1\tilde{E}_A^p][(n_2 + 1)\tilde{E}_B^h + n_2\tilde{E}_B^p] = 0, \quad (4)$$

where $\tilde{E}_{A(B)}^{p(h)} = E_{A(B)}^{p(h)} - \omega$. Three low-lying excitations for the CDW(1/2) are shown in Fig. 3a. The excitations of the MI state can also be obtained from the Eq. (3) by substituting $n_1 = n_2$. At the phase boundaries of the insulating states excitations become gapless and the analytical form of the phase boundaries can also be obtained from Eq. (4) by substituting $\omega = 0$ and $\mathbf{k} = 0$. These are represented by solid lines along with the numerically obtained results in Fig. 1.

In the SF phase, with the ground state values $\bar{f}_n^{(i)}$, one can also get the spectra of the excitations from Eq. (2). These quasiparticles, with mixed particle-hole character, are gapless and have phonon-like linear dispersion (Fig. 3b). Deep in the SF (for large values of t), however, $\bar{f}_n^{(i)}$ obey the Poissonian distribution $\bar{f}_n^{(i)} = \phi_i^n \exp(-|\phi_i|^2/2)/\sqrt{n!}$ and Eq. (2)

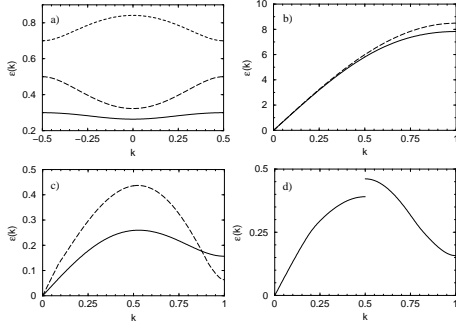


Fig. 3

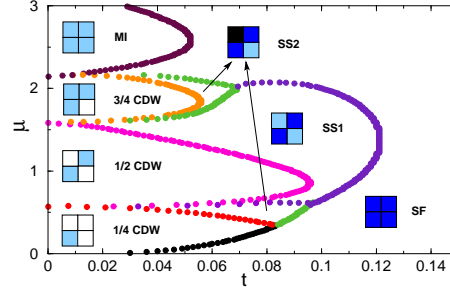


Fig. 4

Fig. 3 – Excitation spectra for $Vd = 0.4$ along $k_x/\pi = k_y/\pi = k$. a) Excitation spectra of CDW ($td = 0.08, \mu = 0.3$), solid line: hole excitation on sublattice A, dashed line: particle excitation on sublattice B, short-dashed line: particle excitation on A b) Spectrum in the deep SF regime (solid line with $td = 2, \mu = 0.4$), dashed line is the excitation spectrum of the effective DNLS for the same parameters. c) solid line: the SF excitation spectrum near SS boundary ($td = 0.17, \mu = 0.4$), dashed line: the SF spectrum close to CDW phase ($t = 0.12, \mu = 0.05$), notice the mode softening near the BZ boundary. d) SS excitation spectrum for $td = 0.16, \mu = 0.4$ (energies are in units of U).

Fig. 4 – Phase diagram of the eBHM in 2D with $V = 0.4$ and $V' = 0.4/(2\sqrt{2})$ (energies are in units of U).

reduces to a discrete nonlinear Schrödinger equation (DNLS):

$$i \frac{\partial \phi_i}{\partial \tau} = -t \sum_{\delta} \phi_{i+\delta} + U |\phi_i|^2 \phi_i + V \sum_{\delta} |\phi_{i+\delta}|^2 \phi_i - \mu \phi_i. \quad (5)$$

In this limit the excitation spectrum can be obtained analytically (dashed line in Fig. 3b) with the sound velocity $[2td(U + 2Vd)|\phi|^2]^{1/2}$ and it matches very well with the numerical result, obtained from Eq. (2). However, as one moves towards the insulating phases, $|\phi|^2$ deviates significantly from ρ , and the description in terms of the DNLS becomes progressively inaccurate. As we approach the MI boundary, ϕ reduces and finally vanishes at the transition point signaling a continuous transition at which a gap opens up for the particle and the hole excitations. This behavior has to be contrasted with the approach towards the modulated phases (SF-CDW and SF-SS) where a mode softening in the SF spectrum at $\mathbf{k} = (\pi, \pi)$ implies the instability of the homogeneous SF phase and appearance of states with broken translational symmetry [19] (Fig. 3c). Once the SS boundary is crossed, we observe a gapless, phonon-like mode in the reduced BZ due to nonvanishing SF fraction, as well as higher energy gapped mode as shown in Fig. 3d. The appearance of the gap can be understood as due to the doubling of the unit cell and the Bragg reflection at $\mathbf{k} = (\pi/2, \pi/2)$.

Let us now discuss the possibility of observing these phases experimentally. The novel, translational symmetry broken phases such as SS and CDW appear because of the longer range interactions between bosons. There are many ways which we could use to achieve bosonic systems with such interactions. One possibility is to use Rydberg atoms; however, they have short life-times that make them difficult candidates to observe these phenomena. The most promising candidate is a dipolar condensate of ^{52}Cr atoms which have a large magnetic dipole moment [1]. A spin-polarized dipolar system, to the leading order, has a power-law tail with $V_{ij} \sim \mu_d^2/|\mathbf{r}_i - \mathbf{r}_j|^3$ where μ_d is the dipole moment and i, j are two lattice

sites. The on-site interaction U can be tuned by Feshbach resonance and t by the intensity of the laser beams which form the optical lattice. Polarization of the dipoles can be manipulated by external magnetic field which can produce repulsive interaction between the atoms. Once such a condensate is formed in an optical lattice and interactions are tuned by external sources, the phases such as the CDW and the SS could be observed in experiments similar to Ref. [2]. Both CDW and SS phases are characterized by modulation of the particle density in real space imaging (since both of them have a crystalline order). In addition the CDW will have a gap in the excitation spectrum. The SS phase will show phase coherence in the time of flight experiments. In particular, we find that momentum distribution $n(\mathbf{k})$ in a $N \times N$ lattice sites is given by:

$$n(\mathbf{k}) = (\rho_A + \rho_B)/2 + (|\phi_A|^2 + |\phi_B|^2)(\alpha_x\alpha_y - 1)/2 + \alpha_x\alpha_y(|\phi_A|^2 \cos(k_x + k_y) + |\phi_B|^2 \cos(k_x - k_y))/2 + \phi_A\phi_B\alpha_x\alpha_y(\cos k_x + \cos k_y) \quad (6)$$

where $\alpha_{x/y} = (2/N) \sin^2(k_{x/y}N/2)/\sin^2(k_{x/y})$. In the SF, $\rho_A = \rho_B$ and $\phi_A = \phi_B$. We see that contrary to the SF case, where the momentum distribution has a sharp central peak, the SS is characterized by additional peaks at $(\pm\pi, \pm\pi)$, (small compared to the central peak) characteristic of the ordering wave-vector of the checkerboard phase. We have checked that the presence of a confining harmonic trap does not destroy the CDW and the SS phases, but leads to coexistence of different phases [20]. Time dependent Gutzwiller theory can be applied to calculate the excitation spectra in trapped systems as well [21].

Finally, we consider the effect of next-nearest neighbor interaction (NNNI), $V' \sum_{i,\delta'} n_i n_{i+\delta'}$, on the phase diagram, where δ' is next-nearest neighbor of site i . In 2D for $V' = V/(2\sqrt{2})$ (relevant for dipolar interaction), we plot the phase diagram in Fig. 4. Checkerboard CDW and SS are formed for $V > 2V'$. In addition new phases appear, such as: CDW with one particle (CDW(1/4)) and three particles (CDW(3/4)) in 2×2 sublattice and SS with three sublattice modulation (SS2) (see Fig. 4). Similar phases can also be obtained by mapping hard-core bosons to Heisenberg spin model with NNNI [16, 22], although the phase diagram is different from the soft-core boson model. In real dipolar gases, the long-range nature of the interaction (which is truncated to NNNI in this work) as well as anisotropy (which is also neglected here) could be important. However, as can be seen from Fig. 4., inclusion of further interactions introduces CDW states of different filling fractions and CDW and SS of different ordering wavevectors; we do not expect fundamentally new phases to appear due to the long-range interaction. It is also clear that striped CDW or SS phases with $(\pi, 0)$ ordering will be absent in real dipolar gases since $2V' < V$. Even for realistic dipolar interactions, with the anisotropy (e.g. an attractive potential along the z -axis when the dipoles are polarized in the $x - y$ plane) included, we expect, for example, CDW and SS phases with $(\pi, \pi, 0)$ wavevector, if a collapsed phase is avoided by having a large on-site repulsion that can be achieved using a Feshbach resonance or alternatively, by having pancake-shaped condensates. This, however, needs further study. Preliminary results indicate that this indeed is happening.

In conclusion, we have studied the lattice bosons with NNI and presented their ground state phase diagram and the low-lying excitations in the four phases, by a time-dependent generalization of the Gutzwiller ansatz. In particular, the SF excitations exhibit a mode softening at the BZ boundary as phases with broken translational symmetry are approached. We also studied the effect of NNNI on the phase diagram of the lattice bosons. We have proposed that such phases could be seen in dipolar condensates and discussed a number of ways to detect them. Recent success in achieving dipolar condensate of ^{52}Cr atoms and manipulating the interactions [1], we believe, could lead to the detection of these interesting

phases, particularly the SS, as well as creation of frustrated lattice bosons [23, 24] and the study of many associated interesting phenomena yet to be explored.

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